Organic Chemistry #1

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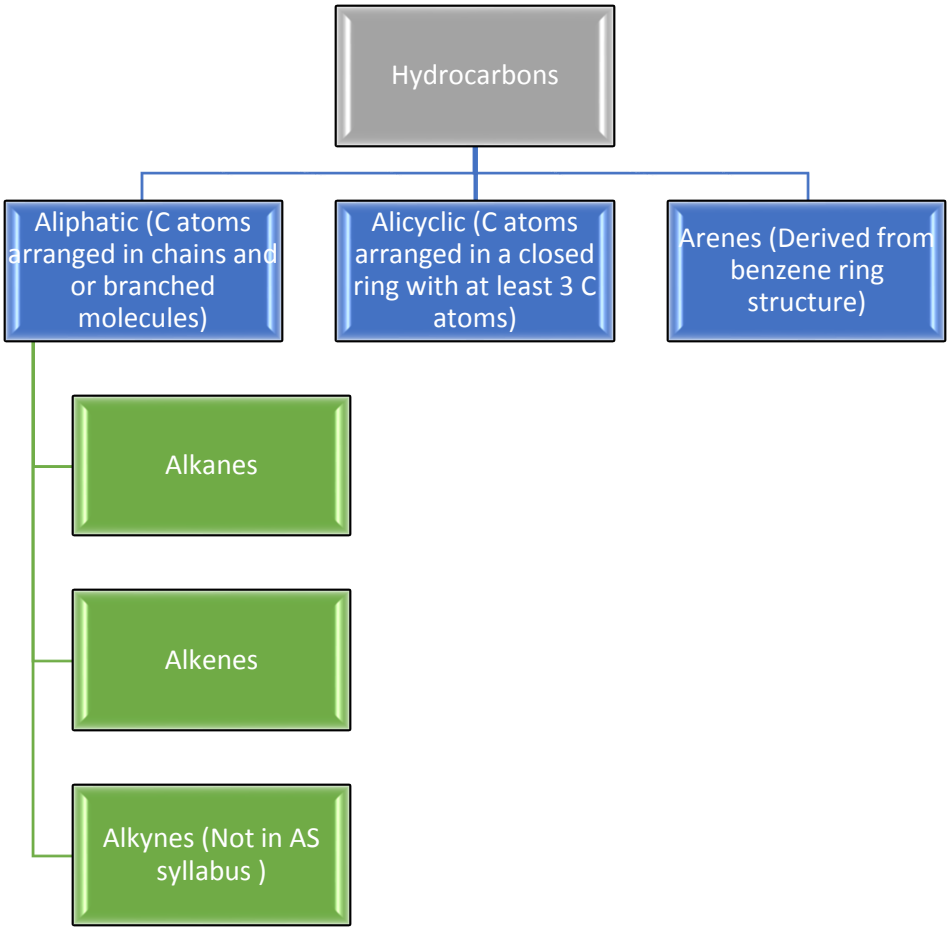
Special thanks to Ms Williams and Ms Matrella for their constant support and inspiration

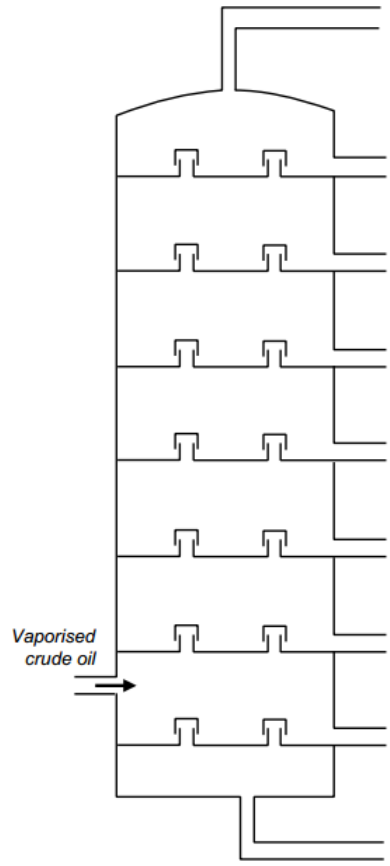
Please note that these guides are a collation of my personal notes, teachers' notes, chemistry books, and websites such as chemguide, chemsheets, chemwiki and wikipedia.

Also note, some of the information in this guide may relate to Unit 1 and Unit 2 Organic Chemistry. I will try to make this as short as :D

Introduction



Crude oil can be split up into fractions by fractional distillation. High boiling fractions may be broken down into useful lower boiling ones - cracking.
Isomerisation produces branched alkanes.
Reforming produces cycloalkanes and arenes.



Approximate boiling range / °C	C's per molecule	Name of fraction	Use(s)
< 25	1 - 4	LPG (Liquefied Petroleum Gas)	*Calor Gas* *Gamping Gas*
40-100	4 - 12	GASOLINE	*Petrol*
100-150	7 - 14	NAPHTHA	*Petrochemicals*
150-200	11 - 15	KEROSINE	*Aviation Fuel*
220-350	15 - 19	GAS OIL	*Central Heating Fuel*
> 350	20 - 30	LUBRICATING OIL	*Lubrication Oil*
> 400	30 - 40	FUEL OIL	*Power Station Fuel* *Ship Fuel*
> 400	40 - 50	WAX, GREASE	*Candles* *Grease for bearings*
> 400	> 50	BITUMEN	*Road surfaces,* *Roofing*

Refining Crude Oil

Fractional Distillation

- Separates the compounds according to their boiling point
- At each level a mixture of compounds in a similar boiling range is taken off
- Rough fractions can then be distilled further to obtain narrower boiling ranges
- Some fractions are more important - usually the lower boiling point ones

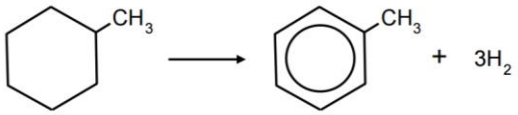
Cracking

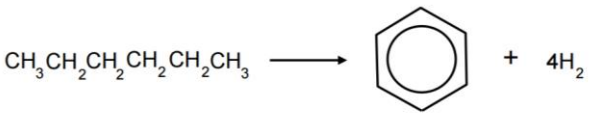
- Involves the breaking of C-C bonds in alkanes
- Converts heavy fractions into higher value products
- Two types:
  - Thermal: Free radical mechanism
  - Catalytic: Carbocation (carbonium ion) mechanism

Reforming

- Converts alkanes to cycloalkanes and cycloalkanes to arenes
- Catalyst: platinum and rhenium
  or platinum and iridium

Examples

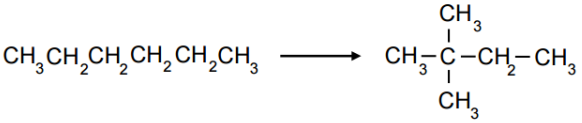




Isomerisation

- Converts straight chain alkanes to branched alkanes using platinum as a catalyst
- Why? Because branched alkanes are used in car engines as combustion is easier and smoother because the molecules break down easier

Example



Hazards & Risks

(Have a read, just in case)

Hazard: The way in which an object or a situation may cause harm
Risk: The chance that harm will actually occur

Hazard Cards

Toxic to humans

Flammable if exposed to ignition sources, sparks, heat. Some substances with this symbol may also give off flammable gases in contact with water

Irritant

Harmful

*Contains gas under pressure. Gas released may be very cold. *Gas container may explode if heated.
*Do not heat containers
*Avoid contact with skin and eyes

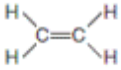
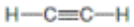
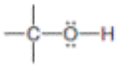
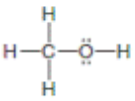
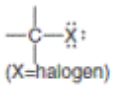
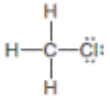
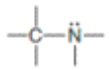
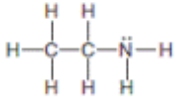
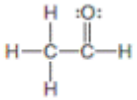
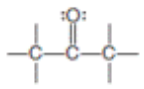
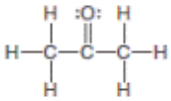
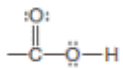
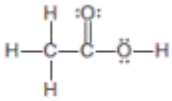
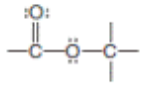
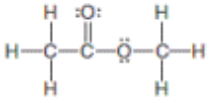
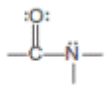
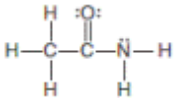
Environmentally Toxic

Can burn readily in air - even without air, or can intensify fire in combustible materials (materials that are easy to ‘catch on fire’).

*May explode if exposed to fire, heat, shock, friction.
*Avoid ignition sources (sparks, flames, heat)
*Keep yourself at a far enough distance for protection/place suitable guard in front of you
*Wear protective clothing

Functional Groups

Table 18.2 Common Functional Groups

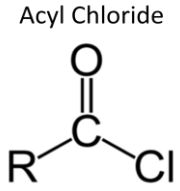
FUNCTIONAL GROUP	COMPOUND TYPE	SUFFIX OR PREFIX OF NAME	EXAMPLE	SYSTEMATIC NAME (COMMON NAME)
	alkene	-ene		ethene (ethylene)
	alkyne	-yne		ethyne (acetylene)
	alcohol	-ol		methanol (methyl alcohol)
 (X=halogen)	haloalkane	halo-		chloromethane (methyl chloride)
	amine	-amine		ethylamine
	aldehyde	-al		ethanal (acetaldehyde)
	ketone	-one		propanone (acetone)
	carboxylic acid	-oic acid		ethanoic acid (acetic acid)
	ester	-oate		methyl ethanoate (methyl acetate)
	amide	-amide		ethanamide (acetamide)

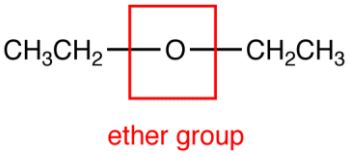
In organic chemistry, a homologous series is a group of organic compounds having the same chemical properties since they have the same functional group

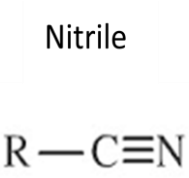
A functional group is a group of atoms responsible for the characteristic reactions of a particular compound.

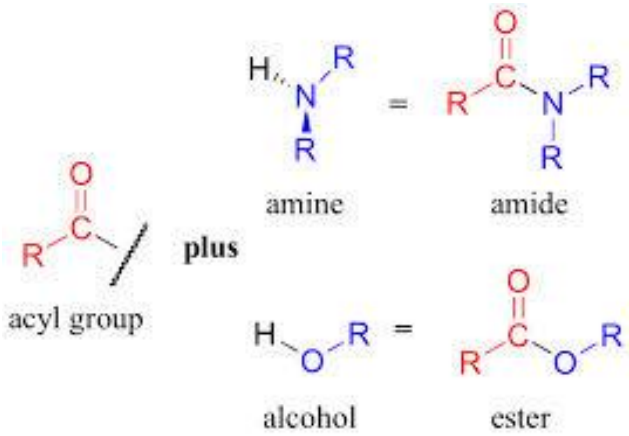
Members of the same homologous series differ in their physics properties (such as density, mp and bp). As the molecular mass increase, the Van der Waals' forces become gradually stronger and gradually increase the mentioned physical properties.

Alkyl group : group of carbon and hydrogen atoms derived from an alkane molecule by removing one hydrogen atom. The name of the alkyl group is derived from the name of its alkane by replacing the - *ane* suffix with - *yl*, e.g., methyl, CH_3, from methane, CH_4, and ethyl, C_2H5 , from ethane, C_2H_6.







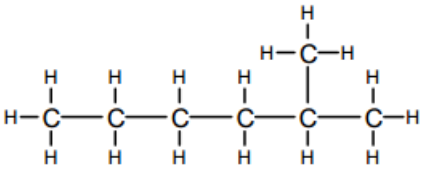


Naming Organic Compounds

The name is based around the name of the longest carbon chain (which contains the functional group):

- The position of the functional group is given by a number counting from the end that gives the lowest number (e.g. but-2-ene, pentan-1-ol, hexan-3-one).
- Add-on groups go at the front of the name (e.g. chloromethane, methylpropane). Note we only include numbers if they are needed.
- Where there are two or more of the same add-on groups, di-, tri- or tetra- are used.
- If there is more than one add-on group, the groups are listed in alphabetical order with numbers (ignoring di, tri, etc.). e.g. 3-bromo-1-chlorobutane, 2,2-dibromo-1 chlorobutane

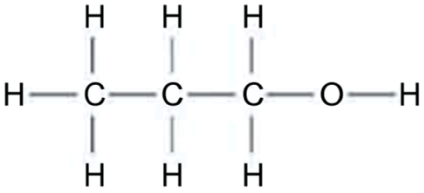
For example:



Longest Chain is 6 Carbons with no C=C double bonds and only one side group (methyl) which is positioned on the 2nd or 4th carbon. We take the smallest number and call it: 2-methyl hexane

Drawing Compounds

There are many ways to represent a compound such as Propan-1-ol:

molecular formula	C_3H_8O
structural formula	$CH_3CH_2CH_2OH$ or $C_2H_5CH_2OH$
displayed formula	

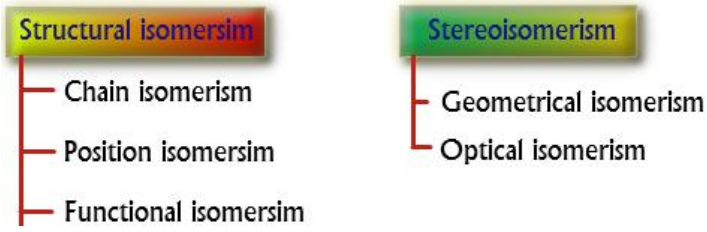
Skeletal formula

When drawing skeletal formulas, you have to consider that each vertex you draw is a carbon except the one in the end if you have a side group attached such as OH, Cl, Br, etc... So using this drawing, the 3 red dots are 3 carbons while the green dot isn't a carbon. The advantage

while using skeletal is that it takes less time to draw as you don't need to draw the Hydrogens connected to the carbons. However you still need to draw any side groups attached to the chain. More can be found on YouTube on how to draw skeletal formulas.

Isomers

Isomers are organic compounds of the same molecular formula but different properties. They can represented.



Chain Isomers

Below is a table that shows the different chain isomers of CH_4 ---> C_6H_{14}

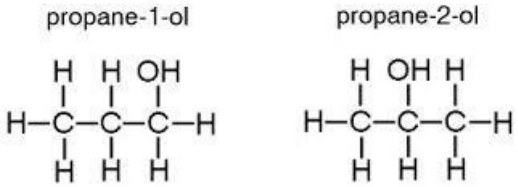
Chain isomers have the same:
-Same molecular formula
-Functional Group
The only difference between them is their chain arrangement.

Alkane	Number of Isomers	Isomers
Methane	1	CH_4 Methane
Ethane	1	C_2H_6 Ethane
Propane	1	C_3H_8 Propane
Butane	2	C_4H_{10} Butane 2-methylpropane $CH_3CH_2(CH_3)CH_3$
Pentane	3	C_5H_{12} Pentane $CH_3CH_2(CH_3)CH_2CH_3$ 2-methylbutane $CH_3C(CH_3)_2CH_3$ 2 2-dimethylpropane
Hexane	5	Hexane 2-methylpentane 3-methylpentane 2,2-dimethylbutane 2,3-dimethylbutane

Positional Isomers

These are isomers of the same:
-Molecular formula
-Functional group

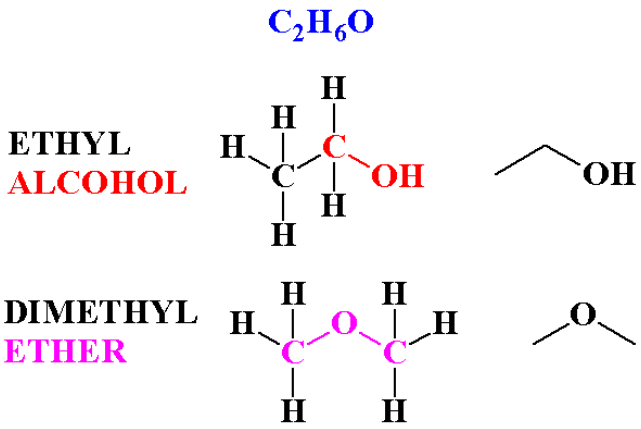
However, their functional group position is different. For example, in the picture below



you can see that the position of the OH side group changes. Another example is when you have an alkene. If the double bond changes it position, e.g. Pent-1-ene to Pent-2-ene, then it is also considered a positional isomer.

Functional Group Isomers

These are isomers of the same molecular formula, yet different functional groups. Even though the isomers belong to different homologous series, they are still said to be isomers - a special type though. In the example shown, both compounds contain 2 Carbons, 6 Hydrogens and one Oxygen. BUT they have different functional groups.

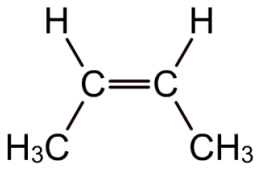


Geometric Isomers

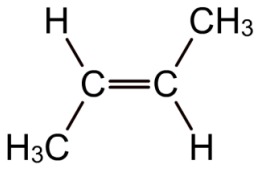
These have same molecular formula and are always **unsaturated** with functional group C=C. This double bond restricts rotation about it.

Cis-trans isomerism:

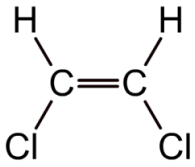
If an alkyl group or atom other than hydrogen is attached to each carbon then the isomers can be named either cis ('on the same side') or trans ('on the opposite side').



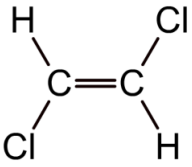
cis-but-2-ene



trans-but-2-ene



cis-1,2-dichloroethene



trans-1,2-dichloroethene

E-Z Isomerism:

IF multiple hydrogen atoms have been substituted by different groups, isomers CANNOT be defined using the cis–trans notation. For example, YOU CANNOT TELL which halogenoalkane is the cis isomer and which is the trans isomer?

Instead, a different system is used for these type of molecules: E–Z notation. Isomers are identified as either E or Z depending on what 'priority' is given to the groups attached to the carbon atoms in the double bond.

'E' represents the German word 'entgegen', and corresponds to trans isomers. The highest priority groups are on the opposite side of the double bond. Remember Enemies are far away.

'Z' represents the German word 'zusammen', and corresponds to cis isomers. The highest priority groups are on the same side of the double bond. Remember friend**z** are close together.

From chemguide:

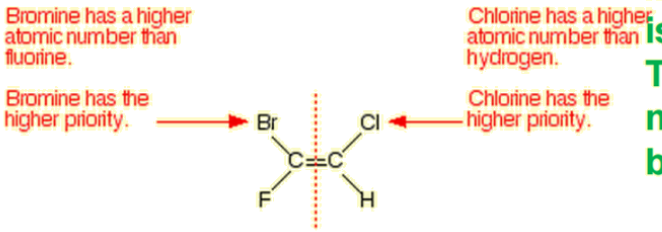
The first rule for very simple cases

You look first at the atoms attached directly to the carbon atoms at each end of the double bond - thinking about the two ends separately.

- The atom which has the higher atomic number is given the higher priority.

Let's look at the example we've been talking about.

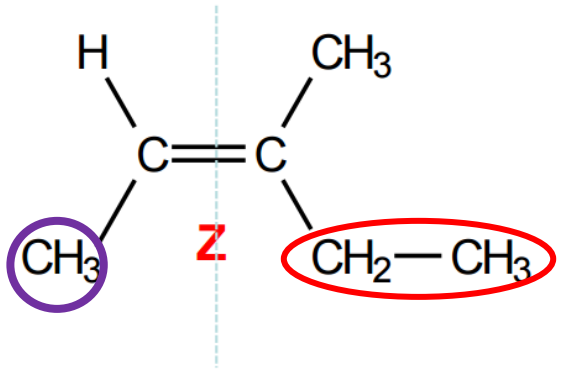
Just consider the first isomer - and look separately at the left-hand and then the right-hand carbon atom. Compare the atomic numbers of the attached atoms to work out the various priorities.



In the naming of this isomer The CIS/TRANS naming method breaks down!

Notice that the atoms with the higher priorities are both on the same side of the double bond. That counts as the (Z)- isomer.

If you have 2 alkyl groups attached to one of the carbons in the double bond, like this:

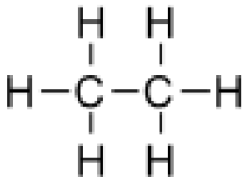


Then consider which alkyl group has a larger mass. In this case it is the ethyl group (in the red circle. Hence the ethyl group gets the priority on the right hand side of the molecule and the methyl (in purple circle) on the left hand side. Hence this is Z-3-methylpent-2-ene.

Alkanes

These are saturated hydrocarbons. They are saturated because no more Hydrogens can bond to the chain. Only single bonds are present in these molecules. The general formula is C_nH_{2n+2}

Here is an example:
An alkane with 2 carbons, hence 6 Hydrogens
Ethane



You also have to know that alkanes are used as fuels and obtained from the fractional distillation, cracking (of long chain alkanes to shorter alkanes) and reformation of crude oil.

When fuels combust they will combust completely if there is excess supply of oxygen to give off CO_2 and water vapour. If there isn't an excess supply of oxygen, the fuel will combust to give off CO (carbon monoxide which is poisonous) and water vapour. You need to be able to balance combustion equations.

Free Radical Substitution

Step 1:
Initiation

This stage require energy from UV light (a possible source is sunlight). In this stage the Cl_2 molecule breaks down to 2 Cl radical. The radical is represented by Cl•. A radical is a species with an unpaired electron.

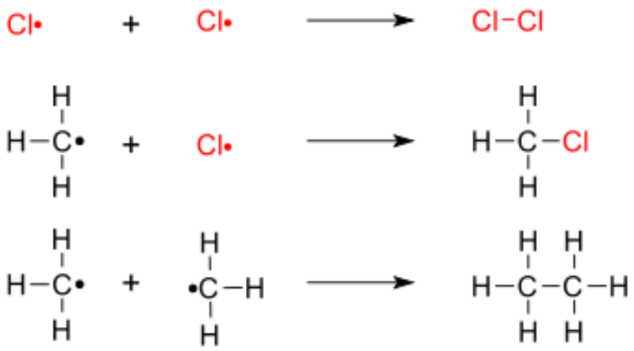
Note the half curly arrow (red arrow) represents the movement of 1 electron while the full curly arrow (black arrow) represents the movement of 2 electrons.

STEP 2: Propagation (Substitution)

THEN...

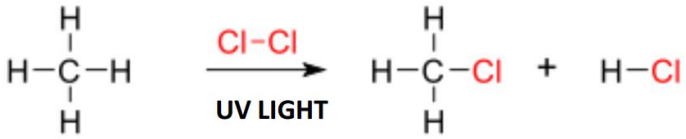
Note how in Initiation, we have 2 radicals on the product side, while in propagation we have 1 radical on each side. Finally in termination we have 2 radicals on the reactants' side.

STEP 3



Termination

OVERALL EQUTATION



$$CH_4 + Cl_2 \xrightarrow{uv\ light} CH_3Cl + HCl$$

Alternative Fuels

(Have a read, no need to memorize full paragraphs)

What is sustainability?

In terms of fuels, it is a fuel which can be renewed (e.g. regrown) within a human lifetime and causes no long-term damage to the environment.

What's wrong with using fossil fuels?

Fossil fuels are non-renewable energy resources. Their supply is limited and they will eventually run out. Fossil fuels do not renew themselves, while fuels such as wood can be renewed endlessly.

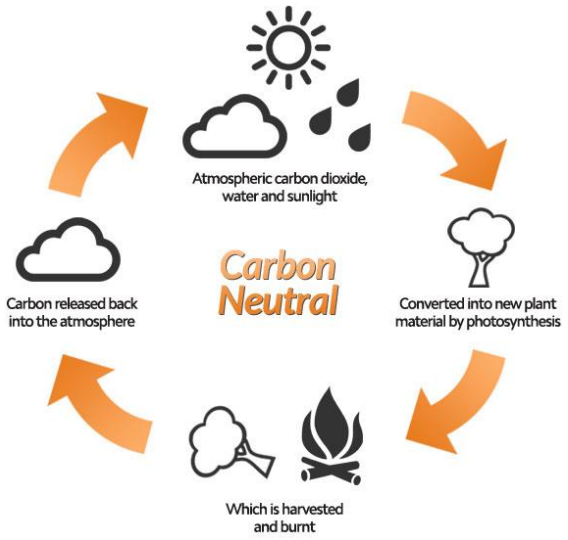
Fossil fuels release carbon dioxide when they burn, which adds to the greenhouse effect and increases global warming. Of the three fossil fuels, for a given amount of energy released, coal produces the most carbon dioxide and natural gas produces the least.

Coal and oil release sulphur dioxide gas when they burn, which causes breathing problems for living creatures and contributes to acid rain.

What does a "carbon neutral" fuel mean?

Carbon neutral is a term used to describe fuels that neither contribute to nor reduce the amount of carbon (measured in the release of carbon dioxide) into the atmosphere.

Pure bio-fuels (i.e. bio-diesel, bio-ethanol and bio-butanol) are carbon neutral since the CO_2 released by being burned is absorbed by plants. In other words, the CO_2 released by burning a gallon of biodiesel today is absorbed from the atmosphere



by soybean plants being grown to produce tomorrow's next gallon. Hence, no net carbon added.

Bio-Fuel

Biodiesel is made from rapeseed oil and other plant oils. It can be used in diesel-powered vehicles without needing any modifications to the engine.

Ethanol, C_2H_5OH, is a liquid fuel that burns well. Bio-ethanol is made by fermenting sugars from sugar cane, wheat and other plants. It cannot be used on its own unless the engine is modified. However, modern petrol engines can use petrol containing up to 10 percent ethanol without needing any modifications.

Ethical Concerns

There are ethical issues surrounding the use of bio-fuels. For example, crops that could be used to feed people are used to provide the raw materials for bio-fuels instead. This could cause food shortages or increases in the price of food. Economic advantages to be considered though include:

- human resources -more people are needed to produce bio-fuels than are needed to produce petrol and diesel, hence more jobs are created
- increased income - for farmers
- lower fuel prices - bio-fuels limit the demand for fossil fuels, helping to reduce increases in fuel prices

There are environmental issues surrounding the use of bio-fuels. Biodiesel naturally contains little sulphur. For example, it may be said that they are carbon neutral ‑ the amount of carbon dioxide released when they are used is the same as the amount absorbed by the plants as they grew. If so, this would reduce the production of this greenhouse gas. However, while bio-fuels produce less carbon dioxide overall, they are not carbon neutral. This is because fossil fuels are used in their production, for example in making fertilisers for the growing plants.

Alkenes

Alkenes have the general formula: C_nH_{2n}
These are unsaturated hydrocarbons. They are called so because some of the bonds between the carbons are double bonds, represented by C=C. If one of these double bonds broke to become a single bond, 2 Hydrogens can be added on to the carbons.

Orbitals overlap when a bond is formed. The carbon-carbon double bond consists of two types of bonds:

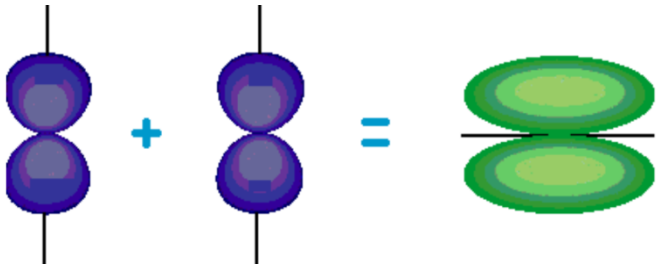
- SIGMA BOND - σ bond – simple overlap of orbitals
- PI BOND π bond – a sideways (lateral) overlap of the orbital above and below the σ bond

Sigma Bond

– In H_2 , two s orbitals overlap
– In CH4 s + p orbitals overlap
– In C2H6 two p orbitals overlap end-to-end
These are known as sigma bonds (σ-bonds)

Pi Bond

The 2 p orbitals overlap sideways (laterally) to produce regions of electron density above and below the axis joining the 2 nuclear centres. This is called a pi bond.



The remaining sections mentioned in the syllabus about alkenes in Unit 1 are covered brilliantly in the Edexcel Chemistry Book from pages 129 - 135. Pages 136 - 141 cover recycling polymers and their problems. If you don't have the book, here is a link: https://www.xtremepapers.com/community/attachments/edexcel-as-chemistry-pdf.14505/

If the link doesn't work or if you have questions or comments please email me: mahtah1@gmail.com